d his

(FILE 'HOME' ENTERED AT 10:39:27 ON 04 JAN 2002)

FILE 'REGISTRY' ENTERED AT 10:39:44 ON 04 JAN 2002

STRUCTURE UPLOADED L1

0 S L1 L2

3 S L1 SSS FULL L3

FILE 'CAPLUS' ENTERED AT 10:41:15 ON 04 JAN 2002

S L1

FILE 'REGISTRY' ENTERED AT 10:41:20 ON 04 JAN 2002

L4

FILE 'CAPLUS' ENTERED AT 10:41:23 ON 04 JAN 2002

L50 S L4

FILE 'CAPLUS' ENTERED AT 10:41:36 ON 04 JAN 2002

2 S L3 L6

2 S L6 L7

SELECT L6 1 RN

FILE 'REGISTRY' ENTERED AT 10:44:00 ON 04 JAN 2002

 $r_8$ 49 S E1-49

FILE 'BEILSTEIN' ENTERED AT 10:46:16 ON 04 JAN 2002

L9 4 S L1

L10 37 S L1 SSS FULL

L11 0 S L10 AND PY<1998

FILE 'STNGUIDE' ENTERED AT 10:50:10 ON 04 JAN 2002

FILE 'MARPAT' ENTERED AT 10:54:39 ON 04 JAN 2002

L120 S L3

L13 6 S L3 SSS FULL

FILE 'CAPLUS' ENTERED AT 10:56:15 ON 04 JAN 2002

L146 S L13

=> s 114 not 16

L15 5 L14 NOT L6

=> d 11

L1 HAS NO ANSWERS

L1STR

Structure attributes must be viewed using STN Express query preparation.

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=> d 1-5 fbib abs
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```
L15 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS
    2001:228892 CAPLUS
AN
DN
    134:266142
    Preparation of 7-acylamino-3-heteroarylthio-3-cephem carboxylic acid
ΤI
    derivatives as antibiotics and prodrugs
IN
    Hecker, Scott J.; Cho, Aesop; Glinka, Tomasz W.; Calkins, Trevor; Lee,
    Ving J.
    Microcide Pharmaceuticals, Inc., USA
PA
SO
    PCT Int. Appl., 199 pp.
    CODEN: PIXXD2
DT
    Patent
LA
    English
FAN.CNT 1
    PATENT NO.
                                        APPLICATION NO. DATE
                    KIND DATE
    ______
                                        ______
PΙ
    WO 2001021623
                     A1
                          20010329
                                        WO 2000-US26069 20000921
        W: AU, BR, CA, CN, CZ, HU, IL, JP, KR, MX, NO, NZ, PL, RO, RU, SG,
            SK, ZA
        RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
            PT, SE
                                        US 1999-155496 P 19990922
OS
    MARPAT 134:266142
GΙ
```

#### \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Antimicrobial (7R)-7-acylamino-3-heteroarylthio-3-cephem-4-carboxylic acid derivs. I and II [R = [(alk1)p(R99)q(alk2)rR12]1-2; R1 = aryl and pyridyl, thiadiazolyl or thiazolyl heterocycles substituted with OH, Br, F, Cl, I,

L15 AN

DN

ΤI

ΙN

PA

SO

DT

LA

ΡI

NO 2001004484

Α

20011026

```
SH, CN, alkylthio, carboxyl, oxo, alkoxycarbonyl, alkyl, alkenyl, nitro,
     amino, alkoxyl and carboxamido; R2 = H, substituted alkyl, alkenyl, aryl,
     aralkyl or trialkylsilyl; R11 = H, halogen, OH, substituted alkyl, alkoxy,
     amino; alk1 and alk2 = alkylene groups; p = 0 or 1; R99 = NH, S, SO, SO2;
     q = 0 or 1; r = 0 or 1; R12 = NR21R22, NR23C(=NR24)NR25R26,
     C(=NR27)NR28R29, NR30CH(=NR31) and R21R31 are independently H and alkyl;
     A, B, D, L, E, G, J are independently N or C forming 3- or 4-pyridyl,
     2-pyrazinyl, 4-pyrimidinyl, 2- or 5-thiazolyl-, 2-1,3,4-thiadiazolyl,
     5-1,2,4-thiadiazolyl] or their pharmaceutically acceptable salts and
     prodrugs were prepd. These cephalosporins were evaluated for
     antimicrobial activity against a panel of bacterial strains and found to
     exhibit antibiotic activity against a wide spectrum of organisms including
     organisms which are resistant to methicillin-resistant bacteria or other
     .beta.-lactam antibiotics and are useful as antibacterial agents with the
     preferred dose of 2.0-250 mg/kg of the patient body wt. administered
     between 1-4 times/day. Thus III was prepd. in good yield starting from
     2-(tert-butoxycarbonyl)aminoethylthiol and 2-bromo-4-chloromethyl-1,3-
     thiazole via a multistep synthesis.
RE.CNT 10
(1) Blank, B; JOURNAL OF MEDICINAL CHEMISTRY 1974, V17(10), P1065 CAPLUS
(2) Ciba Geigy Ag; EP 0022245 A 1981 CAPLUS
(3) Ciba Geigy Ag; EP 0025017 A 1981 CAPLUS
(4) Kim, M; WO 9958535 A 1999 CAPLUS
(5) Merck & Co Inc; WO 9602548 A 1996 CAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT
    ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS
     2000:666701 CAPLUS
     133:252050
     Preparation of novel N-cyanomethyl amide compounds and compositions as
     protease inhibitors to treat osteoporosis
     Bryant, Clifford M.; Palmer, James T.; Rydzewski, Robert M.; Setti,
     Eduardo L.; Tian, Zong-Qiang; Venkatraman, Shankar; Wang, Dan-Xiong
     Axys Pharmaceuticals, Inc., USA
     PCT Int. Appl., 155 pp.
     CODEN: PIXXD2
     Patent
     English
FAN.CNT 2
     PATENT NO.
                      KIND DATE
                                            APPLICATION NO. DATE
                      ____
                            _____
                                            _____
     WO 2000055126
                       A2
                             20000921
                                            WO 2000-US6837
                                                             20000315
     WO 2000055126
                            20010222
                       A3
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             CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV,
             MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG,
             SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW,
             AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                            US 1999-124420 P 19990315
     EP 1161415
                       A2
                            20011212
                                            EP 2000-916375
                                                             20000315
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO
                                            US 1999-124420 P 19990315
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WO 2000-US6837 W 20000315

20010914

NO 2001-4484

US 1999-124420 P 19990315 WO 2000-US6837 W 20000315

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PATENT FAMILY INFORMATION:
    2000:666700
                                          APPLICATION NO. DATE
     PATENT NO.
                     KIND DATE
                           _____
                                          -----
     WO 2000055125
                   A2
                           20000921
                                          WO 2000-US6747 20000315
PΙ
                     A3
     WO 2000055125
                          20010426
            AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
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             IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV,
             MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG,
             SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW,
             AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
             DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
             CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                          US 1999-124420 P 19990315
     NO 2001004485
                      Α
                           20011105
                                          NO 2001-4485
                                                           20010914
                                          US 1999-124420 P 19990315
                                          WO 2000-US6747 W 20000315
OS
     MARPAT 133:252050
     Title compds. [R1R2NCR3R4CN; R1 = R11R7NCR5R9X1,
AΒ
     R11R8NCR6R10X2NR7CR5R9CX1; X1, X2 independently = CO, CH2SO2; R5, R6
     independently = H, C1-6alkyl; R7, R8 independently = H, C1-6alkyl; R9, R10
     independently = (un)substituted-C1-6alkyl; R9-R7 = trimethylene,
     tetramethylene, phenylene-1,2-dimethylene; R10-R8 = trimethylene,
     tetramethylene, phenylene-1,2-dimethylene; R5-R9 = C3-8cycloalkylene,
     C3-8heterocycloalkylene; R10-R6 = C3-8cycloalkylene, C3-
     8heterocycloalkylene; R11 = X4X5R18; X4 = CO, COCO, SO2; X5 = bond, O, NH;
     R18 = C1-6alkyl; R2 = H, C1-6alkyl; R3 = H, C1-6alkyl; R4 = CN, COOH,
     COOC1-6alkyl; R2-R4 = trimethylene, tetramethylene, phenylene-1,2-
     dimethylene; R4-R3 = C3-8cycloalkylene, C3-8heterocycloalkylene], N-oxide,
     prodrug, isomers, pharmaceutically acceptable salts, and compn. are prepd.
     as therapeutically effective estrogen receptor agonist. Title compds. are
     claimed in treating osteoporosis in post-menopausal woman in which
     cathepsin K activity contributes to the pathol. and symptomatol. of the
     disease. Thus, the title compd. (S)-C6H5CH2OCONHCH(CH2CH(CH3)2)CONHCH2CN
     was prepd.
L15
    ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS
     2000:666700 CAPLUS
AN
DN
     133:252170
TI
     Preparation of novel N-cyanomethyl amides as protease inhibitors
TN
     Bryant, Clifford M.; Bunin, Barry A.; Kraynack, Erica A.; Patterson, John
PA
     Axys Pharmaceuticals, Inc., USA
SO
     PCT Int. Appl., 137 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 2
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                    KIND DATE
                                          APPLICATION NO. DATE
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                           ----<del>-</del>
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                    A2
PΙ
     WO 2000055125
                           20000921
                                          WO 2000-US6747 20000315
     WO 2000055125
                     А3
                          20010426
            AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
             CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID,
             IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV,
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MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG,

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SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW,
               AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
          RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                                  US 1999-124420 P 19990315
     NO 2001004485
                                20011105
                                                  NO 2001-4485
                                                                    20010914
                          Α
                                                  US 1999-124420 P 19990315
                                                  WO 2000-US6747 W 20000315
PATENT FAMILY INFORMATION:
     2000:666701
FAN
                                                  APPLICATION NO.
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     WO 2000055126
                         A2
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                                                  WO 2000-US6837 20000315
PT
      WO 2000055126
                         А3
                                20010222
               AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
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               IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV,
               MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG,
               SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
          RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
               CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                                  US 1999-124420 P 19990315
                          A2 20011212
      EP 1161415
                                                  EP 2000-916375 20000315
          R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
               IE, SI, LT, LV, FI, RO
                                                  US 1999-124420 P 19990315
                                                  WO 2000-US6837 W 20000315
     NO 2001004484
                                 20011026
                                                  NO 2001-4484
                          Α
                                                                  20010914
                                                  US 1999-124420 P 19990315
                                                  WO 2000-US6837 W 20000315
OS
     MARPAT 133:252170
GΙ
             R1 CN CN R4
                                                                  II
                           III
                                                                  IV
```

AB The title compds. [I; R1 = II, III (wherein X1, X2 = CO, CH2SO2; R5, R6 = H, alkyl; R7, R8 = H, alkyl, etc.; R9, R10 = alkyl optionally substituted with CN, halo, NO2, etc.; R11 = X5X6R18; X5 = CO, COCO, SO2; X6 = a bond, O, NH, N(alkyl); R18 = alkyl optionally substituted with CN, halo, NO2, etc.); R2 = H, alkyl, etc.; R3 = H, alkyl, etc.; R4 = H, alkyl optionally

PA

SO

Laboratories Upsa, Fr.

Fr. Demande, 28 pp.

substituted with CN, halo, NO2, etc.; R4 and R2 taken together form trimethylene, tetramethylene, phenylene-1,2-dimethylene, optionally substituted with hydroxy, oxo or methylene; R4 and R3 together with the carbon atom to which both are attached form cycloalkylene, heterocycloalkylene], useful for treating diseases assocd. with cysteine protease activity, particularly diseases assocd. with activity of cathepsins B, K, L or S such as inflammation and asthma, were prepd. and formulated. Thus, reacting 2(S)-tert-butoxycarbonylamino-3-phenylpropionic acid with aminoacetonitrile.HCl in the presence of Et3N in DMF and MeCN afforded the amide (1S)-IV. Biol. data for compds. I were given.

```
L15 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2002 ACS
ΑN
    2000:666699 CAPLUS
DN
     133:251875
ΤI
     Preparation of esters as protease inhibitors
IN
     Buysse, Ann M.; Mendonca, Rohan V.; Palmer, James T.; Tian, Zong-Qiang;
     Venkatraman, Shankar
    Axys Pharmaceuticals, Inc., USA
PA
     PCT Int. Appl., 108 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
    English
FAN.CNT 1
     PATENT NO.
                    KIND DATE
                                         APPLICATION NO. DATE
                     ____
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                                          -----
                   A2
                                         WO 2000-US7145 20000315
PI
    WO 2000055124
                           20000921
     WO 2000055124
                     A3 20010816
            AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU,
            CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID,
            IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV,
            MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG,
            SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW,
            AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,
            DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF,
            CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                                          US 1999-124529 P 19990315
     EP 1159260
                      A1
                          20011205
                                          EP 2000-918085
                                                           20000315
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO
                                          US 1999-124529 P 19990315
                                          WO 2000-US7145 W 20000315
OS
    MARPAT 133:251875
     R1X1NR2CHR3COR4 [X1 = bond or divalent group; R1 = H, X6X7R16; R2 = H,
AB
     alkyl; R3 = H, optionally substituted alkyl; R2R3 = trimethylene,
     tetramethylene, phenylene-1,2-dimethylene; R4 = nitromethyl,
     1-hydroxy-1-methylethyl, etc.], cysteine protease inhibitors, were prepd.
     E.g., benzyl 1S-(3-hydroxy-2-oxo-1S-phenethylpropylcarbamoyl)-3-
     methylbutylcarbamate was prepd. The test compds. were inhibitors of
     cathepsin B, K, L, and S (no data).
L15
    ANSWER 5 OF 5 CAPLUS COPYRIGHT 2002 ACS
ΑN
     1994:134290 CAPLUS
DN
     120:134290
     Preparation of .alpha.-(sulfonylamino)-N-(4-pyridyl)benzenepropanamides
ΤI
     and their pharmaceutical formulations as analgesics
     Bru-Magniez, Nicole; Sartori, Eric; Teulon, Jean Marle
ΙN
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CODEN: FRXXBL

DT Patent LA French FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE							
ΡI	FR 2683817	A1	19930521	FR 1991-14187	19911118							
	FR 2683817	B1	19940225									

OS MARPAT 120:134290

GΙ

AB Title compds. racemic or (R)- or (S)-I [R = C1-18 alkyl, C3-7 cycloalkyl, haloalkyl, AR' (A = bond or C1-6 (un)satd. aliph. chain, R' = (substituted) Ph or naphthyl, (substituted) heteroaryl of 5-7 atoms contg. 1-3 heteroatoms (N, O, or S)); R1 = H, lower alkyl; R2 = H, halo] are prepd. Thus, sulfonylation of .alpha.-amino deriv. (S)-II (prepn. given) with MeSO2Cl in THF with added K2CO3 afforded (S)-I (R1 = R2 = H, R = Me). Compds. I are useful as analgesics. Thus, compd. (S)-I (R1 = 3-Me, R2 = H, R = Me) was effective in inhibition of the torsion and stretching movement induced by phenylbenzoquinone in mice (ID50 = 2.8 mg kg-1). Pharmaceutical formulations of compds. I are claimed.

#### > d 1-2 fbib abs hitstr

```
L6 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS
```

AN 1999:736655 CAPLUS

DN 131:351230

TI Method for stereochemically controlled preparation of isomerically pure highly substituted azacycloalkanamines and -ols

IN Reggelin, Michael; Heinrich, Timo; Junker, Bernd; Antel, Jochen; Preuschoff, Ulf

PA Solvay Pharmaceuticals G.m.b.H., Germany

SO PCT Int. Appl., 72 pp.

CODEN: PIXXD2

DT Patent

LA German

FAN.CNT 1

LAU.						KIND DATE			APPLICATION NO. DATE									
PI	WO				A1 19991118				WO 1999-DE1417 19990510									
		W:												-	CH,	-	-	
														-	IL,	-	-	-
			•	•	•	•		•		•	•	•	•	,	MD,		•	•
			-		-	•	•	•	•	•	•	-	•		SK,		•	•
						UG,	US,	UΖ,	VN,	YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	KΖ,	MD,
		DW.	•	TJ,		TC	MTAT	g D	СТ	C 7	ПС	77.7	יח ע	יזמ	CU	CV	שם	DV
		KW:						-	-	-		•			CH, BF,	•	•	•
												TD,		эш,	Dr,	υ,	Cr,	cu,
			01, 0	011,	011,	OIV,	OW, 1	1111,	1111,	•	•	•		418A	199	8051 <sup>-</sup>	3	
	DE 19921580			A1 19991125				DE 1998-19821418A 19980513 DE 1999-19921580 19990510										
								DE 1998-19821418A119980513										
	ΑU	AU 9950250		Al 19991129														
								DE 1998-19821418A 19980513										
								WO 1999-DE1417 W 19990510										
	BR	9911	9911770		A 20010206			BR 1999-11770 19990510										
								DE 1998-19821418A 19980513										
								WO 1999-DE1417 W 19990510										
	EP				A1 20010221 CH, DE, DK, ES,													
		R:	•	•	•	•	•	ES,	FR,	GB,	GR,	ΙТ,	LI,	LU,	NL,	SE,	PT,	IE,
			SI,	LT,	LV,	FΊ,	RO			D	E 10	00 1	0001	4107	100	0051	2	
									DE 1998-19821418A 19980513 WO 1999-DE1417 W 19990510									
	NΟ	2000005666		A 20001110														
	110	2000003000			A 20001110				DE 1998-19821418A 19980513 WO 1999-DE1417 W 19990510									
										•••						0		

OS CASREACT 131:351230; MARPAT 131:351230

Ι

GI

mis appli.

II

AB Title compds. [I; R = OH or NH2; R1 = H, alkyl, (un) substituted Ph; R2 = H

H; R1R2 = [alkyl- or (un) substituted Ph-substituted] CH2; R3 = H; R4 = H, alkyl, (un) substituted phenylalkyl; R3R4 = alk(en) ylene; R7 = H; R8 = H, alkyl, Co2H, CONH2, heterocyclyl, etc.; R9 = H, alkyl, phenylalkyl, etc.; R8R9 = alkylene] were prepd. using chiral S-alkenylarylsulfoximides. Thus, (+)-(RS)-(4R)-4-isopropyl-2-(p-tolyl)-4,5dihydro[1,2.lambda.6,3]oxathiazole 2-oxide was condensed with BrMgCH2CH: CHMe and the product O-protected to give (R)-Me2CHCH(CH2OSiMe3)N:S(0)(C6H4Me-4)CH2CH:CHMe which was cyclocondensed with N-protected MeCHCH2CH(NH2)CHO (prepn. given) to give, in 1 addnl. step, title compd. (+)-(2S, 3S, 4S, 5S)-II.

ΙT 250613-41-3P

> RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(method for stereochem. controlled prepn. of isomerically pure highly substituted azacycloalkanamines and -ols)

RN 250613-41-3 CAPLUS

1-Pyrrolidinecarboxylic acid, 3-hydroxy-5-[[(R)-N-[(1R)-1-(1-R)-1]]]CN hydroxymethyl)-2-methylpropyl]-S-(4-methylphenyl)sulfonimidoyl]methyl]-4methyl-2-(2-methylpropyl)-, 1,1-dimethylethyl ester, (2S,3S,4S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RE.CNT 11 RE

- (1) Beak, P; J Org Chem 1993, V58(5), P1109 CAPLUS
- (2) Ciba Geigy Ag; EP 0558443 A 1993 CAPLUS
- (3) Comins, D; Heterocycles 1994, V37(2), P1121 CAPLUS
- (4) Fujisawa Pharmaceutical Co; EP 0394991 A 1990 CAPLUS
- (5) Meleshina, A; 1974, 23, CAPLUS
- ALL CITATIONS AVAILABLE IN THE RE FORMAT
- L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS
- AN1998:745666 CAPLUS
- DN 130:95445
- Metalated 2-Alkenylsulfoximides in asymmetric synthesis: TIdiastereoselective preparation of highly substituted pyrrolidine derivatives
- ΑU Reggelin, Michael; Heinrich, Timo
- Fachbereich Chemie Universitat, Frankfurt/Main, D-60439, Germany CS voil barian
- SO Angew. Chem., Int. Ed. (1998), 37(20), 2883-2886 CODEN: ACIEF5; ISSN: 1433-7851
- PB Wiley-VCH Verlag GmbH
- DTJournal
- LА English

GΙ

AB The stereoselective synthesis of enantiomerically pure, highly substituted pyrrolidine derivs. I and II (R1 = H, Me; R2 = CH2Ph, CH2CHMe2, CH2OCMe3) starting from valine-derived alkenylsulfoximides III (p-Tol = 4-MeC6H4) and their enantiomers is described. Thus, lithiation of III, followed by transmetalation with ClTi(OCHMe2)3 and reaction with 9-fluorenylmethoxycarbonyl (Fmoc)-protected .alpha.-amino aldehydes, piperidine-promoted deprotection, cyclization, re-protection with Boc2O, and desulfuration with SmI2 in MeOH gave heterocycles I. The abs. configuration at the newly formed stereogenic centers C-3 and C-4 is controlled by the abs. configuration at sulfur, and the configuration at C-5 is a result of conformational preferences of the cyclization precursor.

### IT 219321-56-9P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(diastereoselective prepn. of highly substituted pyrrolidine derivs. via stereoselective aldol reactions of alkenylsulfoximide titanium anions with protected amino aldehydes)

RN 219321-56-9 CAPLUS

CN 3-Pyrrolidinol, 5-[[(S)-N-[(1S)-1-(hydroxymethyl)-2-methylpropyl]-S-(4-methylphenyl)sulfonimidoyl]methyl]-4-methyl-2-(2-methylpropyl)-, (2S,3R,4R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

#### 219321-41-2P

ΙT

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (diastereoselective prepn. of highly substituted pyrrolidine derivs. via stereoselective aldol reactions of alkenylsulfoximide titanium anions with protected amino aldehydes)

RN 219321-41-2 CAPLUS

CN 1-Pyrrolidinecarboxylic acid, 3-hydroxy-5-[[(S)-N-[(1S)-1-(hydroxymethyl)-2-methylpropyl]-S-(4-methylphenyl)sulfonimidoyl]methyl]-4-methyl-2-(phenylmethyl)-, 1,1-dimethylethyl ester, (2S,3R,4R,5S)- (9CI) (CA INDEX NAME)

# 09/700278

# Absolute stereochemistry.

RE.CNT 40

RE

- (3) Bax, A; J Am Chem Soc 1986, V108, P2093 CAPLUS
- (5) Bridges, R; Bioorg Med Chem Lett 1993, V3, P115 CAPLUS
  (6) Cheung, H; Biochim Biophys Acta 1973, V293, P451 CAPLUS
  (8) Deprez, P; Tetrahedron: Asymmetry 1991, V2, P1189 CAPLUS
  (9) Dess, D; J Am Chem Soc 1991, V113, P7277 CAPLUS

- ALL CITATIONS AVAILABLE IN THE RE FORMAT



8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

Absolute stereochemistry. Rotation (+).

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):48

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IN 1-Pyrrolidinecarboxylic acid, 3-hydroxy-5-methyl-2-(2-methylpropyl)-,
1,1-dimethylethyl ester, (2S,3R,5R)- (9CI)

MF C14 H27 N O3

Absolute stereochemistry. Rotation (+).

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Sulfoximine, N-[(1S)-1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-methylpropyl]-S-methyl-S-(4-methylphenyl)-, [S(S)]- (9CI)

MF C19 H35 N O2 S Si

Absolute stereochemistry.

09/700278

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

Absolute stereochemistry. Rotation (+).

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Sulfoximine, S-(1-cyclopenten-1-ylmethyl)-N-[(1R)-1-[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-methylpropyl]-S-(4-methylphenyl) , [S(R)]- (9CI)
MF C24 H41 N O2 S Si

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C27 H30 N2 O4

Absolute stereochemistry.

$$\bigcap_{N \in \mathbb{R}} O$$

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Cyclopenta[c]pyrrole-2(1H)-carboxylic acid, 3a-aminohexahydro-1-methyl-3phenyl-, 1,1-dimethylethyl ester, (1R,3S,3aR,6aR)- (9CI)

Ĺ

MF C19 H28 N2 O2

Absolute stereochemistry. Rotation (+).

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L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Sulfoximine, N-[(1R)-1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2methylpropyl]-S-methyl-S-(4-methylphenyl)-, [S(S)]- (9CI)
MF C19 H35 N O2 S Si

Absolute stereochemistry. Rotation (+).

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Cyclopenta[c]pyrrole-2(1H)-carboxylic acid, hexahydro-3a-hydroxy-1-methyl3-phenyl-, 1,1-dimethylethyl ester, (1R,3S,3aR,6aR)- (9CI)
MF C19 H27 N O3

Absolute stereochemistry. Rotation (+).

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2.lambda.4-1,2,3-Oxathiazole, 4,5-dihydro-4-(1-methylethyl)-2-(4-methylphenyl)-, 2-oxide, (2R,4R)- (9CI)
MF C12 H17 N O2 S

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Cyclopenta[c]pyrrol-3a(1H)-ol, 1-[[[S-(S)]-N-[(1R)-1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-methylpropyl]-S-(4-methylphenyl)sulfonimidoyl]methyl]hexahydro-3-phenyl-, (1S,3S,3aR,6aR)-(9CI)

MF C32 H50 N2 O3 S Si

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Pyrrolidinecarboxylic acid, 2-[(1,1-dimethylethoxy)methyl]-3-hydroxy-5methyl-, 1,1-dimethylethyl ester, (2S,3S,5S)- (9CI)
MF C15 H29 N O4

Absolute stereochemistry. Rotation (+).

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C21 H23 N O3

Absolute stereochemistry.

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Cyclopenta[c]pyrrole-2(1H)-carboxylic acid, 1-[[[S(R)]-N-[(1R)-1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-methylpropyl]-S-(4-methylphenyl)sulfonimidoyl]methyl]hexahydro-3a-hydroxy-3-phenyl-, 1,1-dimethylethyl ester, (1R,3S,3aS,6aS)- (9CI)
MF C37 H58 N2 O5 S Si

Absolute stereochemistry. Rotation (-).

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Pyrrolidinecarboxylic acid, 3-hydroxy-4,5-dimethyl-2-(phenylmethyl)-,
1,1-dimethylethyl ester, (2S,3S,4S,5S)- (9CI)

MF C18 H27 N O3

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 2.lambda.4-1,2,3-Oxathiazole, 4,5-dihydro-4-(1-methylethyl)-2-(4-methylphenyl)-, 2-oxide, (2R,4S)- (9CI)
MF C12 H17 N O2 S

Absolute stereochemistry.

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Pyrrolidinecarboxylic acid, 3-hydroxy-5-[[(R)-N-[(1R)-1-(1-hydroxymethyl)-2-methylpropyl]-S-(4-methylphenyl)sulfonimidoyl]methyl]-4-methyl-2-(2-methylpropyl)-, 1,1-dimethylethyl ester, (2S,3S,4S,5R)- (9CI)

MF C27 H46 N2 O5 S

Absolute stereochemistry. Rotation (-).

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

#### 09/700278

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IN 1-Pyrrolidinecarboxylic acid, 3-hydroxy-5-methyl-2-(phenylmethyl)-,
1,1-dimethylethyl ester, (2S,3S,5S)- (9CI)

MF C17 H25 N O3

Absolute stereochemistry. Rotation (+).

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Benzeneethanol, .beta.-amino-, (.beta.S)- (9CI)

MF C8 H11 N O

CI COM

Absolute stereochemistry. Rotation (+).

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Sulfoximine, S-2-butenyl-N-[(1R)-1-(1-hydroxymethyl)-2-methylpropyl]-S-(4-methylphenyl)-, [S(R)]- (9CI)

MF C16 H25 N O2 S

Absolute stereochemistry. Double bond geometry unknown.

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Pyrrolidinecarboxylic acid, 3-hydroxy-4,5-dimethyl-2-(2-methylpropyl)-,
1,1-dimethylethyl ester, (2S,3R,4R,5R)- (9CI)

MF C15 H29 N O3

Absolute stereochemistry.

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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IN Cyclopentanone (8CI, 9CI)

MF C5 H8 O

CI COM

## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C14 H25 N O3

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Pyrrolidinecarboxylic acid, 2-[(1,1-dimethylethoxy)methyl]-3-hydroxy-5methyl-, 1,1-dimethylethyl ester, (2S,3R,5R)- (9CI)

MF C15 H29 N O4

Absolute stereochemistry. Rotation (+).

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN L-Leucine (9CI)

MF C6 H13 N O2

CI COM

Absolute stereochemistry. Rotation (+).

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C15 H21 N O

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Pyrrolidinecarboxylic acid, 3-hydroxy-5-methyl-2-(phenylmethyl)-,
1,1-dimethylethyl ester, (2S,3R,5R)- (9CI)

MF C17 H25 N O3

Absolute stereochemistry. Rotation (-).

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

MF C23 H19 N O3

Absolute stereochemistry.

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Pyrrolidinecarboxylic acid, 2-[(1,1-dimethylethoxy)methyl]-3-hydroxy-4,5dimethyl-, 1,1-dimethylethyl ester, (2S,3S,4S,5S)- (9CI)

MF C16 H31 N O4

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN Sulfoximine, S-(1-cyclopenten-1-ylmethyl)-N-[(1R)-1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-methylpropyl]-S-(4-methylphenyl)-, [S(S)]- (9CI)
MF C24 H41 N O2 S Si

Absolute stereochemistry. Rotation (+).

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

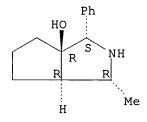
L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS
IN 1H-Isoindole-1,3(2H)-dione, 2-[(1R,3S,3aR,6aR)-hexahydro-1-methyl-3-phenylcyclopenta[c]pyrrol-3a(1H)-yl]- (9CI)
MF C22 H22 N2 O2

Absolute stereochemistry.

09/700278

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

Absolute stereochemistry. Rotation (-).



## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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IN Sulfoximine, N-[(1R)-1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2 methylpropyl]-S-methyl-S-(4-methylphenyl)-, [S(R)]- (9CI)
MF C19 H35 N O2 S Si

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Cyclopenta[c]pyrrole-2(1H)-carboxylic acid, 1-[[[S-(S)]-N-[(1R)-1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-methylpropyl]-S-(4-methylphenyl)sulfonimidoyl]methyl]hexahydro-3a-hydroxy-3-phenyl-, 1,1-dimethylethyl ester, (1S,3S,3aR,6aR)- (9CI)
MF C37 H58 N2 O5 S Si

Absolute stereochemistry. Rotation (+).

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Cyclopenta[c]pyrrole-2(1H)-carboxylic acid, hexahydro-3a-hydroxy-1-methyl3-phenyl-, 1,1-dimethylethyl ester, (1S,3S,3aS,6aS)- (9CI)
MF C19 H27 N O3

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2.lambda.4-1,2,3-Oxathiazole, 4,5-dihydro-4-(1-methylethyl)-2-(4-methylphenyl)-, 2-oxide, (2S,4R)- (9CI)

MF C12 H17 N O2 S

Absolute stereochemistry.

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

Absolute stereochemistry. Rotation (-).

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Pyrrolidinecarboxylic acid, 3-hydroxy-4,5-dimethyl-2-(2-methylpropyl)-,
1,1-dimethylethyl ester, (2S,3S,4S,5S)- (9CI)

MF C15 H29 N O3

Absolute stereochemistry. Rotation (+).

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2.lambda.4-1,2,3-Oxathiazole, 4,5-dihydro-4-(1-methylethyl)-2-(4-methylphenyl)-, 2-oxide, (2S,4S)- (9CI)

MF C12 H17 N O2 S

Absolute stereochemistry. Rotation (-).

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Cyclopenta[c]pyrrol-3a(1H)-ol, 1-[[[S(R)]-N-[(1R)-1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-methylpropyl]-S-(4-methylphenyl)sulfonimidoyl]methyl]hexahydro-3-phenyl-, (1R,3S,3aS,6aS)-(9CI)

MF C32 H50 N2 O3 S Si

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Pyrrolidinecarboxylic acid, 3-hydroxy-5-methyl-2-(2-methylpropyl)-,
1,1-dimethylethyl ester, (2S,3S,5S)- (9CI)

MF C14 H27 N O3

Absolute stereochemistry. Rotation (-).

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Carbamic acid, [(1S)-1-(hydroxymethyl)-3-methylbutyl]-,
9H-fluoren-9-ylmethyl ester (9CI)

MF C21 H25 N O3

Absolute stereochemistry.

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN Sulfoximine, S-2-butenyl-S-(4-methylphenyl)-N-[(1R)-2-methyl-1-[(trimethylsilyl)oxy]methyl]propyl]-, [S(R)]- (9CI)

MF C19 H33 N O2 S Si

Absolute stereochemistry.

Double bond geometry unknown.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Pyrrolidinecarboxylic acid, 2-[(1,1-dimethylethoxy)methyl]-3-hydroxy-4,5dimethyl-, 1,1-dimethylethyl ester, (2S,3R,4R,5R)- (9CI)

MF C16 H31 N O4

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2-Butene, 1-bromo- (6CI, 7CI, 8CI, 9CI)

MF C4 H7 Br

CI COM

Br-CH2-CH=CH-CH3

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 2(1H)-Isoquinolinecarboxylic acid, octahydro-4a-hydroxy-1-methyl-, 1,1-dimethylethyl ester, (1R,4aS,8aR)- (9CI)

MF C15 H27 N O3

Absolute stereochemistry. Rotation (-).

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1-Pyrrolidinecarboxylic acid, 3-hydroxy-4,5-dimethyl-2-(phenylmethyl)-,
1,1-dimethylethyl ester, (2S,3R,4R,5R)- (9CI)

MF C18 H27 N O3

# 09/700278

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L8 49 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 1H-Isoindole-1,3(2H)-dione (9CI)

MF C8 H5 N O2

CI COM

## L10 ANSWER 1 OF 37 COPYRIGHT 2002 BEILSTEIN CDS MDLI

Beilstein Reg. No. (BRN): 8180518 Beilstein Molecular Formula (MF): C30 H44 N2 O5 S

Beilstein Reference (SO): 6-21

General Comments (NTE): Stereo compound

Rltd. Stereoisomers (RSI): 8180517 Formula Weight (FW): 544.75

Lawson Number (LN): 25073; 5224; 3151; 1762; 318

# Preparation:

PRE

Start: BRN=8178275 C25H36N2O3S, BRN=1911173 tert-butyl carbonic anhydride

Reag: NaHCO3

Solv: dioxane, H2O

Reference(s):

1. Reggelin, Michael; Heinrich, Timo, Angew.Chem.Int.Ed.Engl., 37 <1998>

20, 2883-2886, LA: EN, CODEN: ACIEAY

Angew.Chem., 110 <1998>, 3005-3008, LA: EN, CODEN: ANCEAD